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A FAST METHOD FOR COMPUTING THE INTEGRALS OF THE RELATIVISTIC COMPTON SCATTERING KERNEL FOR RADIATIVE TRANSFER

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A Fast Method for Computing the Integrals of the Relativistic Compton Scattering Kernel for Radiative Transfer

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For various computer simulation applications, one needs the integrals of the Compton scattering kernel over its parameters. An efficient and accurate method for evaluating these integrals is described and the corresponding software is available upon request.

1. Introduction

In an earlier paper,[1] we presented a simple and fast method for computing the relativistic Compton scattering kernel for radiative transfer. For various code applications, we require integrals of the Compton scattering kernel over various combinations of its parameters. We describe an efficient method for calculating the single integrals over $\xi \equiv \vec{\Omega}\cdot\vec{\Omega}'$ and $\gamma' \equiv h\nu'/(m_0c^2)$, the double integral over ξ and γ' and the triple integral over ξ ,$\gamma \equiv h\nu/(m_0c^2)$ and γ', where γ, $\vec{\Omega}$ (γ', $\vec{\Omega}'$) is the incoming (outgoing) photon energy (in units of electron rest energy m_0c^2) and direction, respectively. The integrals are over an arbitrary, user-specified interval in each of the integration variables.

The essence of the method is to make use of the following inequality derived in Ref. 1:

$$1 \le \frac{\sigma_s(\gamma\to\gamma',\xi,\tau)}{[\Sigma_0\frac{\tau\gamma\gamma'}{q}]} \le 2+4\gamma\gamma', \tag{1}$$

where $\sigma_s(\gamma\to\gamma',\xi,\tau)$ is the Compton scattering kernel,

$$\Sigma_0 \equiv \frac{N_e r_0^2}{4\gamma\nu\tau K_2(\tau^{-1})}e^{-\frac{\lambda_+}{\tau}},$$

$$\tau \equiv kT_e/(m_0c^2)\ ,$$

$$q \equiv \sqrt{\gamma^2+\gamma'^2-2\gamma\gamma'\xi}\ ,$$

$$\lambda_+ \equiv (\frac{\gamma'-\gamma}{2})+\{[1+\gamma\gamma'\frac{(1-\xi)}{2}][1+\frac{(\gamma-\gamma')^2}{2\gamma\gamma'(1-\xi)}]\}^{\frac{1}{2}}.$$

Here, K_2 is the modified Bessel function of the second kind, k is Boltzmann's constant, T_e is the electron temperature, r_0 is the classical electron radius and N_e is the electron density. This simple algebraic expression, which agrees with the Compton scattering kernel to within a factor of order 1, may be used to determine those regions where significant contributions to the integral occur and one need only integrate over these regions. This procedure increases the speed and assures the accuracy of the algorithm.

2. General Considerations

As was pointed out in Ref. 1, the essential features of σ_s are contained in $[\Sigma_0\tau\gamma\gamma'/q]$, particularly in the $\exp(-\lambda_+/\tau)$ factor. Everything else is smoothly varying compared to this exponential except at the point $\gamma' = \gamma$, $\xi = 1$, where $q \to 0$. Therefore, for any given integration region, the integrand peaks near the minimum of λ_+ within the region. Our approach is to find this minimum and then to integrate over only a few e-foldings of $\exp(-\lambda_+/\tau)$ in its vicinity. The following properties of λ_+ are useful in finding this minimum.

First, we hold γ and γ' fixed and seek a minimum in ξ. We write λ_+ in the form

$$\lambda_+ = \frac{1}{2}\{\gamma'-\gamma+[4+(\gamma-\gamma')^2+2|\gamma-\gamma'|(z+\frac{1}{z})]^{\frac{1}{2}}\}, \tag{2}$$

where

$$z = \gamma\gamma'(1-\xi)/|\gamma-\gamma'|.$$

Clearly, we are at a minimum in ξ only if z=1 or

$$\xi = 1-|\gamma-\gamma'|/(\gamma\gamma'). \tag{3}$$

For z=1 and $\gamma' \le \gamma$, we have $\lambda_+ = 1$, while for $\gamma' \ge \gamma$, we have $\lambda_+ = 1+\gamma'-\gamma$.

Next, we hold γ and ξ fixed and seek a minimum in γ'. Setting the first derivative of λ_+ with respect to γ' equal to zero and squaring to get rid of the square root, we find

$$[\gamma-\gamma'-\gamma\gamma'(1-\xi)]\ [\gamma'-\gamma-\gamma\gamma'(1-\xi)]\ [(\gamma+\gamma')^2+(\gamma\gamma')^2(1-\xi)] = 0. \tag{4}$$

The third factor can never be 0 with $\xi^2 \le 1$. The second factor is a root of the squared equation but not of the first derivative. The first factor,

$$\gamma' = \gamma/[1+\gamma(1-\xi)], \tag{5}$$

is the only possible minimum and at that minimum, $\lambda_+ = 1$.

Finally, we hold γ' and ξ fixed and seek a minimum in γ. Setting the first derivative of λ_+ with respect to γ equal to zero, we find, as above, that

$$\gamma = \gamma'/[1-\gamma'(1-\xi)], \tag{6}$$

is the only possible minimum and $\lambda_+ = 1$ at that minimum. If $1-\gamma'(1-\xi) \le 0$, then, for all $\gamma \ge 0$, λ_+ is monotonically decreasing as γ increases.

In the vicinity of the point $\gamma' = \gamma$, $\xi = 1$, the Compton scattering kernel is singular and behaves like

$$\frac{e^{\frac{|\gamma-\gamma'|}{\tau\sqrt{2\gamma^2(1-\xi)}}}}{\sqrt{(\gamma-\gamma')^2+2\gamma^2(1-\xi)}}. \tag{7}$$

If we integrate over γ' for fixed ξ, there is no problem in the vicinity of $\gamma' = \gamma$ even for ξ very near 1. Since the region of physical interest is $\tau<1$, the e-folding width of the exponential is narrower than the width of the peak due to $1/q$, so when we integrate over only a few e-foldings of the exponential we automatically resolve the $1/q$ peak. Numerical integration will be correct if we use $\xi=1-\varepsilon$, where ε is very small but larger than the machine round-off error. This procedure prevents divide-by-zero hardware errors.

If we integrate over ξ for fixed γ', then for $\gamma' = \gamma$ we have an integrable $1/\sqrt{1-\xi}$ singularity. We use as our integration variable $\eta = \sqrt{1-\xi}$, so that

$$\int \sigma_s d\xi = -2\int \sigma_s \eta\, d\eta, \tag{8}$$

and we use a second-order Simpson's rule assuming $\sigma_s\eta$ is quadratic in η between integration points. This change of variables eliminates the singularity.

3. Integral over ξ only

We seek the integral of σ_s over the interval $\underline{\xi} \le \xi \le \overline{\xi}$. For fixed γ and γ', we have shown that the only minimum of λ_+ is at

$$\xi_m = 1-|\gamma-\gamma'|/(\gamma\gamma').$$

Thus, the minimum of λ_+ within the interval occurs at

$$\xi_M = \max[\underline{\xi},\min(\overline{\xi},\xi_m)]. \tag{9}$$

To calculate the integral, we determine $\lambda_{+m1} = \lambda_+(\gamma,\gamma',\xi_M)$ and then determine the e-folding intervals by solving

$$\lambda_{+m1}+n\tau = \lambda_+(\gamma,\gamma',\xi),$$

for ξ, where n=1,2,3.... Within each e-folding interval we use a second-order Simpson's rule and keep doubling the number of integration points till the desired accuracy is reached. The number of e-folding intervals is determined by either reaching the boundary or else when the contribution of the last e-folding interval is less than the acceptable error. The integrand values are determined by calling the Compton scattering kernel subroutine described in Ref. 1.

As was shown in Sec. 2, numerical integration in the vicinity of $\gamma=\gamma'$, $\xi=1$ will be correct if we use $\eta = \sqrt{1-\xi}$ as our integration variable, which eliminates the $1/q$ singularity.

4. Integral over γ' only

The integration interval is $\underline{\gamma}' \leq \gamma' \leq \overline{\gamma}'$. For fixed γ and ξ, we have shown that the only minimum of λ_+ is at

$$\gamma'_m = \gamma/[1+\gamma(1-\xi)].$$

Thus, the minimum of λ_+ within the interval occurs at

$$\gamma'_M = \max[\underline{\gamma}',\min(\overline{\gamma}',\gamma'_m)]. \tag{10}$$

To calculate the integral, we determine $\lambda_{+m1} = \lambda_+(\gamma,\gamma'_M,\xi)$ and then find the e-folding intervals by solving

$$\lambda_{+m1}+n\tau = \lambda_+(\gamma,\gamma',\xi)$$

for γ', where n=1,2,3.... Within each e-folding interval, we use a second-order Simpson's rule and keep doubling the number of integration points till the desired accuracy is reached. The number of e-folding intervals is determined by either reaching the boundary or else when the last e-folding interval's contribution is less than the desired accuracy. The integrand values are determined by calling the Compton scattering kernel subroutine described in Ref. 1.

We use γ' as our integration variable. As was shown in Sec. 2, numerical integration in the vicinity of $\gamma=\gamma'$, $\xi=1$ will be correct if we just use $\xi=1-\varepsilon$, where ε is very small but larger than machine round off error.

5. Integral over ξ and γ'

Let the integration intervals be $\underline{\gamma}' \leq \gamma' \leq \overline{\gamma}'$ and $\underline{\xi} \leq \xi \leq \overline{\xi}$. We do the γ' integral first by calling the subroutine described in the previous section, and then the ξ integral. For fixed ξ, the subroutine described in the previous section will find λ_{+m1}, the minimum of λ_+ within the interval $\underline{\gamma}' \leq \gamma' \leq \overline{\gamma}'$ and integrate over only a few e-foldings of $\exp(-\lambda_+/\tau)$ in its vicinity. We then need to find the minimum of λ_{+m1} over all ξ in the interval $\underline{\xi} \leq \xi \leq \overline{\xi}$, and integrate over only a few e-foldings of $\exp(-\lambda_{+m1}/\tau)$ in its vicinity.

The largest contribution to the integral comes from those values of ξ for which λ_{+m1} is 1. For a given ξ, the minimum of λ_+ in the interval is 1 only if

$$\underline{\gamma}' \leq \gamma/[1+\gamma(1-\xi)] \leq \overline{\gamma}'$$

or, equivalently,

$$\underline{\xi}_m \leq \xi \leq \overline{\xi}_m\,, \tag{11}$$

where

$$\underline{\xi}_m = 1+1/\gamma-1/\underline{\gamma}' \text{ and } \overline{\xi}_m = 1+1/\gamma-1/\overline{\gamma}'.$$

Thus, our first integration subregion is $\max(\underline{\xi},\underline{\xi}_m) \le \xi \le \min(\overline{\xi},\overline{\xi}_m)$ and if this interval is not empty, we set $\lambda_{+m2} = 1$.

If $\overline{\xi}_m \le \overline{\xi}$, then, for all $\xi \ge \overline{\xi}_m$,

$$\overline{\gamma}' \le \gamma/[1+\gamma(1-\xi)] \le \gamma\,,$$

so for these values of ξ, $\lambda_{+m1} = \lambda_+(\gamma,\overline{\gamma}',\xi)$. The minimum value of λ_{+m1} is at

$$\xi = 1-|\gamma-\overline{\gamma}'|/(\gamma\overline{\gamma}') = \overline{\xi}_m\,, \tag{12}$$

since $\overline{\gamma}' \le \gamma$. Therefore, the minimum value of λ_{+m1} in the intersection of the integration interval and $\xi \ge \overline{\xi}_m$, occurs at $\max(\overline{\xi}_m,\underline{\xi})$ and we call this λ_{+m2} and then determine the e-folding intervals in ξ by solving

$$\lambda_{+m2}+n\tau = \lambda_+(\gamma,\overline{\gamma}',\xi)$$

for ξ, where n=1,2,3.... This determines our second set of integration subregions.

If $\underline{\xi} \le \underline{\xi}_m \le 1$, then, for all $\xi \le \underline{\xi}_m$,

$$\gamma/[1+\gamma(1-\xi)] \le \underline{\gamma}',$$

so for these values of ξ, $\lambda_{+m1} = \lambda_+(\gamma,\underline{\gamma}',\xi)$. The minimum value of λ_{+m1} is at

$$\xi = 1-|\gamma-\underline{\gamma}'|/(\gamma\underline{\gamma}') = \underline{\xi}_m\,, \tag{13}$$

since $\underline{\xi}_m \le 1$ implies $\underline{\gamma}' \le \gamma$. Therefore, the minimum value of λ_{+m1} in the intersection of the integration interval and $\xi \le \underline{\xi}_m$, occurs at $\min(\underline{\xi}_m,\overline{\xi})$ and we call this λ_{+m2} and then determine the e-folding intervals in ξ by solving

$$\lambda_{+m2}+n\tau = \lambda_+(\gamma,\underline{\gamma}',\xi)$$

for ξ, where n=1,2,3.... This determines our third set of integration subregions.

If $1 \le \underline{\xi}_m$, then, for all $\xi \le \underline{\xi}_m$,

$$\gamma/[1+\gamma(1-\xi)] \le \underline{\gamma}',$$

so for these values of ξ, $\lambda_{+m1} = \lambda_+(\gamma,\underline{\gamma}',\xi)$. The minimum value of λ_{+m1} is at

$$\xi = 1-|\gamma-\underline{\gamma}'|/(\gamma\underline{\gamma}') = 2-\underline{\xi}_m\,, \tag{14}$$

since $1 \le \underline{\xi}_m$ implies $\gamma \le \underline{\gamma}'$. Therefore, the minimum value of λ_{+m1} in the integration interval occurs at $\max[\underline{\xi},\min(\overline{\xi},2-\underline{\xi}_m)]$ and we call this λ_{+m2} and then determine the e-folding intervals in ξ by solving

$$\lambda_{+m2}+n\tau = \lambda_+(\gamma,\underline{\gamma}',\xi)$$

for ξ, where n=1,2,3.... This determines our fourth set of integration subregions.

As was shown in Sec. 2, numerical integration in the vicinity of γ=γ', ξ=1 will be correct if we just use $\eta = \sqrt{1-\xi}$ as our integration variable which eliminates the $1/q$ singularity. This is important for the case where $|\underline{\gamma}'-\gamma|$ and $|\overline{\gamma}'-\gamma|$ are both small and $\overline{\xi} = 1$. Within each integration subregion we use a second-order Simpson's rule and keep doubling the number of integration points till the desired accuracy is reached. The number of e-folding intervals is determined by either reaching the boundary ($\underline{\xi}$ or $\overline{\xi}$) or else when the contribution of the last e-folding subregion is less than the acceptable error. The integrand values are determined by calling the subroutine described in the previous section.

6. Integrate over ξ, γ' and average over γ

Let the integration intervals be $\underline{\gamma} \le \gamma \le \overline{\gamma}$, $\underline{\gamma}' \le \gamma' \le \overline{\gamma}'$ and $\underline{\xi} \le \xi \le \overline{\xi}$. We integrate over γ' and ξ first by calling the subroutine described in the previous section, and then integrate over γ. For fixed γ, the subroutine described in the previous section will find λ_{+m2}, the minimum of λ_+ within the rectangle $\underline{\gamma}' \le \gamma' \le \overline{\gamma}'$ and $\underline{\xi} \le \xi \le \overline{\xi}$, and integrate over only a few e-foldings of $\exp(-\lambda_+/\tau)$ in its vicinity. We then need to find the minimum of λ_{+m2} over all γ in the interval $\underline{\gamma} \le \gamma \le \overline{\gamma}$, and integrate over only a few e-foldings of $\exp(-\lambda_{+m2}/\tau)$ in its vicinity.

The largest contribution to the integral comes from those values of γ for which λ_{+m2} is 1. For a given γ, the minimum of λ_+ in the rectangle is 1 only if

$$\underline{\gamma}' \le \gamma/[1+\gamma(1-\xi)] \le \overline{\gamma}', \text{ with } \underline{\xi} \le \xi \le \overline{\xi}$$

or, equivalently, since

$$\gamma/[1+\gamma(1-\xi)]$$

is monotonically increasing for $\underline{\xi} \le \xi \le \overline{\xi}$, the minimum of λ_+ in the rectangle is 1 only if

$$\underline{\gamma}' \le \gamma/[1+\gamma(1-\overline{\xi})] \text{ and } \gamma/[1+\gamma(1-\underline{\xi})] \le \overline{\gamma}'.$$

This result is true if and only if

$$\underline{\gamma}_m \le \gamma \le \overline{\gamma}_m\,, \tag{15}$$

where

$$\underline{\gamma}_m = \underline{\gamma}'/\max[+0,1-\underline{\gamma}'(1-\overline{\xi})] \text{ and } \overline{\gamma}_m = \overline{\gamma}'/\max[+0,1-\overline{\gamma}'(1-\underline{\xi})].$$

Thus, our first integration subregion is $\max(\underline{\gamma},\underline{\gamma}_m) \le \gamma \le \min(\overline{\gamma},\overline{\gamma}_m)$.

If $\overline{\gamma}_m \le \overline{\gamma}$, then, for all $\gamma \ge \overline{\gamma}_m$, $\overline{\gamma}' \le \gamma$ and $1-\overline{\gamma}'(1-\underline{\xi}) \ge 0$. Therefore,

$$\overline{\gamma}' \le \gamma/[1+\gamma(1-\underline{\xi})] \le \gamma/[1+\gamma(1-\xi)] \text{ with } \underline{\xi} \le \xi \le \overline{\xi},$$

so the minimum of λ_+ is always at $\overline{\gamma}'$. Furthermore,

$$\gamma \ge \overline{\gamma}'/[1-\overline{\gamma}'(1-\underline{\xi})] \text{ implies } \underline{\xi} \ge 1-(\gamma-\overline{\gamma}')/(\gamma\overline{\gamma}'),$$

which is where the minimum of λ_+ over ξ occurs. Therefore, for these values of γ, $\lambda_{+m2} = \lambda_+(\gamma,\overline{\gamma}',\underline{\xi})$, and as was shown in Sec. 2, the minimum value of λ_{+m2} is at

$$\gamma = \overline{\gamma}'/[1-\overline{\gamma}'(1-\underline{\xi})] = \overline{\gamma}_m\,. \tag{16}$$

Therefore, the minimum value of λ_{+m2} in the intersection of the integration interval and $\gamma \ge \overline{\gamma}_m$, occurs at $\max(\overline{\gamma}_m,\underline{\gamma})$ and we call this λ_{+m3} and then determine the *e*-folding intervals in γ by solving

$$\lambda_{+m3}+n\tau = \lambda_+(\gamma,\overline{\gamma}',\underline{\xi}),$$

for γ, where n=1,2,3.... This determines our second set of integration subregions.

If $\underline{\gamma} \le \underline{\gamma}_m$, then, for all $\gamma \le \underline{\gamma}_m$ and for any $\xi \le 1$,

$$\underline{\gamma}' \ge \gamma/[1+\gamma(1-\xi)]$$

so $\lambda_{+m1} = \lambda_+(\gamma,\underline{\gamma}',\xi)$. Now the minimum of λ_{+m1} over ξ occurs at

$$1-|\gamma-\underline{\gamma}'|/(\gamma\underline{\gamma}')$$

and is 1 if $\gamma \ge \underline{\gamma}'$ and $1+\underline{\gamma}'-\gamma$ if $\underline{\gamma}' \ge \gamma$. Therefore,

$$\text{for } \left\{\begin{array}{c} \underline{\gamma}'/[1+\underline{\gamma}'(1-\overline{\xi})] \le \gamma \le \underline{\gamma}'/\max(0,1-\underline{\gamma}'(1-\overline{\xi})) \\ \underline{\gamma}'/[1+\underline{\gamma}'(1-\underline{\xi})] \le \gamma \le \underline{\gamma}'/[1+\underline{\gamma}'(1-\overline{\xi})] \\ \gamma \le \underline{\gamma}'/[1+\underline{\gamma}'(1-\underline{\xi})] \end{array}\right\}, \text{ we have}$$

$$\left\{\begin{array}{c} \overline{\xi} \le 1-|\gamma-\underline{\gamma}'|/(\gamma\underline{\gamma}') \le 1, \text{ and } 1 \le \lambda_{+m2}(\gamma) = \lambda_+(\gamma,\underline{\gamma}',\overline{\xi}) \le 1+\underline{\gamma}'-\underline{\gamma}'/[1+\underline{\gamma}'(1-\overline{\xi})] \\ \underline{\xi} \le 1-|\gamma-\underline{\gamma}'|/(\gamma\underline{\gamma}') \le \overline{\xi}, \text{ and } 1+\underline{\gamma}'-\underline{\gamma}'/[1+\underline{\gamma}'(1-\overline{\xi})] \le \lambda_{+m2}(\gamma) = 1+\underline{\gamma}'-\gamma \le 1+\underline{\gamma}'-\underline{\gamma}'/[1+\underline{\gamma}'(1-\underline{\xi})] \\ 1-|\gamma-\underline{\gamma}'|/(\gamma\underline{\gamma}') \le \underline{\xi}, \text{ and } 1+\underline{\gamma}'-\underline{\gamma}'/[1+\underline{\gamma}'(1-\underline{\xi})] \le \lambda_{+m2}(\gamma) = \lambda_+(\gamma,\underline{\gamma}',\underline{\xi}) \end{array}\right\}. \tag{17}$$

Here, $\lambda_{+m2}(\gamma)$ decreases monotonically as γ increases in each of these three intervals, so the minimum value of $\lambda_{+m2}(\gamma)$ is at $\gamma = \underline{\gamma}_m$. Therefore, the minimum value of $\lambda_{+m2}(\gamma)$ in the intersection of the integration interval and $\gamma \le \underline{\gamma}_m$, occurs at $\min(\underline{\gamma}_m,\overline{\gamma})$ and we call this λ_{+m3} and then determine the *e*-folding intervals in γ by solving

$$\lambda_{+m3}+n\tau = \lambda_{+m2}(\gamma),$$

for γ, where n=1,2,3.... This determines our third set of integration subregions.

Within each integration subregion, we use a second-order Simpson's rule and keep doubling the number of integration points till the desired accuracy is reached. The number of e-folding intervals is determined by either reaching the boundary ($\underline{\gamma}$ or $\overline{\gamma}$) or else when the last e-folding subregion's contribution is less than the acceptable error. The integrand values are determined by calling the subroutine described in the previous section.

7. Conclusion

These subroutines were checked by comparing them with the nonrelativistic Thomson cross sections, the results of Matteson[2] and the results of Wienke.[3] We obtained good agreement in all cases. These routines are available from the author.

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